

```
chain nodes :
   19 21 22
ring nodes :
   1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
chain bonds :
   2-22 11-21 13-19
ring bonds :
   1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 12-13 13-14
   13-15 14-17 14-18 15-16 16-17 17-18
exact/norm bonds :
   2-22 5-7 6-10 7-8 7-11 8-9 8-14 9-10 11-12 11-21 12-13 13-14 13-15 14-17
   14-18 15-16 16-17 17-18
exact bonds :
   13-19
normalized bonds :
   1-2 1-6 2-3 3-4 4-5 5-6
G1:0, F, Cl, Br, I
```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 21:CLASS

Match level :

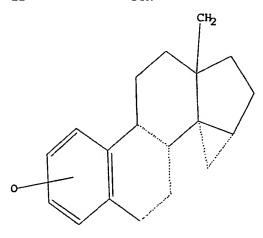
=> Uploading 09937723.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 ST



Structure attributes must be viewed using STN Express query preparation.

6 ANSWERS

=> s 11 sss sam

SAMPLE SEARCH INITIATED 16:10:19 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2028 TO ITERATE

49.3% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 37860 TO 43260

PROJECTED ANSWERS: 34 TO 452

L2 6 SEA SSS SAM L1

Uploading 09937723.str

L3 STRUCTURE UPLOADED

=> d 13

L3 HAS NO ANSWERS

L3 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 13 sss sam

G1 O, F, Cl, Br, I

SAMPLE SEARCH INITIATED 16:14:41 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 705 TO ITERATE

100.0% PROCESSED 705 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 12508 TO 15692

PROJECTED ANSWERS: 2 TO 124

2 SEA SSS SAM L3

=> s 13 sss ful

FULL SEARCH INITIATED 16:15:19 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 14537 TO ITERATE

100.0% PROCESSED 14537 ITERATIONS 16 ANSWERS

SEARCH TIME: 00.00.02

16 SEA SSS FUL L3 L5

=> s 15

1 L5 L6

=> d l6 bib,ab,hitstr

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
L6
AN
     2000:706441 CAPLUS
DN
     133:267019
     Procedure for the production of equilenin derivatives and medicaments
TI
     containing them
IN
     Schwarz, Sigfrid; Thieme, Ina; Undeutsch, Bernd; Kaufmann, Guenter;
     Roemer, Wolfgang
     Jenapharm G.m.b.H. und Co. K.-G., Germany
PA
SO
     Ger. Offen., 8 pp.
     CODEN: GWXXBX
DT
     Patent
     German
LA
FAN.CNT 1
     PATENT NO.
                       KIND DATE
                                             APPLICATION NO. DATE
                       ____
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PT
     DE 19915576
                      A1
                              20001005
                                             DE 1999-19915576 19990330
     WO 2000059922
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                                             WO 2000-EP2513
                       A1
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             CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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              CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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                        Ε
     JP 2002541154
                        T2
                              20021203
                                              JP 2000-609432
                                                                20000322
PRAI DE 1999-19915576
                        Α
                              19990330
     WO 2000-EP2513
                        W
                              20000322
     CASREACT 133:267019; MARPAT 133:267019
os
AB
     New equilenin derivs. I (R1 = H, C1-5-alkyl, C1-5-acyl, COPh; R2 = H; R2R6
     = 0; R3 = H, Me; R4 = H; R4R8 = O, CH2, halomethylene, dihalomethylene; R5
     = H, Me; R6 = H, F, OH, C1-5-acyloxy; R8 = OH, C1-11-acyloxy) as well as
     procedures for their prodn. and formulations of medicaments contg. them
     are described. Thus, 11.alpha.-Hydroxy-3-methoxy-14.alpha.,15.alpha.-
     methyleneestra-1,3,5(10)-trien-17.alpha.-yl acetate (I; R1 = Me, R2 = R8 =
     .beta.-H, R3 = R5 = H, R4 = .alpha.-OAc, R6 = .alpha.-OH) was prepd. from
     3-Methoxy-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),8-tetraen-17.alpha.-
     yl acetate via treatment of 11.alpha.-Hydroxy-3-methoxy-
     14.alpha.,15.alpha.-methylene-8.alpha.,9.alpha.-oxidoestra-1,3,5(10)-trien-
     17.alpha.-yl acetate with P2I4 and pyridien in CHCl3. I exhibit estrogen
     effectiveness and are applicable in hormone therapy with women and men.
     298705-65-4P, 11.alpha.-Hydroxy-3-methoxy-14.alpha.,15.alpha.-
     methylene-8.alpha., 9.alpha.-oxidoestra-1, 3,5(10)-trien-17.alpha.-yl
     acetate 298705-66-5P, 3-Methoxy-14.alpha.,15.alpha.-methylene-
     8.alpha.,9.alpha.-oxidoestra-1,3,5(10)-triene-11.alpha.,17.alpha.-diyl
     diacetate
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
         (prepn. of equilenin derivs. and medicaments contg. them for hormone
        replacement therapy)
RN
     298705-65-4 CAPLUS
CN
     Cycloprop[14,15]estra-1,3,5(10)-triene-11,17-diol, 8,9-epoxy-3',15-dihydro-
```

3-methoxy-, 17-acetate, (8.alpha.,11.alpha.,14R,15.beta.,17.alpha.)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-66-5 CAPLUS

CN Cycloprop[14,15]estra-1,3,5(10)-triene-11,17-diol, 8,9-epoxy-3',15-dihydro-3-methoxy-, diacetate, (8.alpha.,11.alpha.,14R,15.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 298705-67-6P, 3-Methoxy-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),6,8-pentaene-11.alpha.,17.alpha.-diyl diacetate 298705-68-7P, 11.alpha.-Hydroxy-3-methoxy-14.alpha.,15.alpha.methyleneestra-1,3,5(10)-trien-17.alpha.-yl acetate 298705-69-8P , 14.alpha., 15.alpha.-Methyleneestra-1, 3, 5(10), 6, 8-pentaene-3,11.beta.,17.beta.-triol 298705-70-1P, 11.beta.,17.beta.-Dihydroxy-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),6,8-pentaen-3-yl benzoate 298705-71-2P, 11.beta., 17.beta.-Dihydroxy-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),6,8-pentaen-3-yl propionate 298705-72-3P, 3,11.beta.-Dihydroxy-14.alpha.,15.alpha.methyleneestra-1,3,5(10),6,8-pentaen-17.beta.-yl decanoate 298705-73-4P, 3,11.beta.-Dihydroxy-14.alpha.,15.alpha.methyleneestra-1,3,5(10),6,8-pentaen-17-one 298705-74-5P, 3-Methoxy-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),6,8-pentaene-11.alpha.,17.beta.-diyl diacetate 298705-75-6P, 15.beta.-Methyl-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),6,8-pentaene-3,11.beta.,17.beta.-triol 298705-76-7P, 11.beta.-Fluoro-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),6,8-pentaene-3,17.beta.-diol 298705-77-8P, 3,17.beta.-Dihydroxy-14.alpha.,15.alpha.methyleneestra-1,3,5(10),6,8-pentaen-11-one 298705-78-9P, 3-Methoxy-14.alpha.,15.alpha.-methylene-11-oxoestra-1,3,5(10),6,8-pentaen-17.alpha.-yl acetate 298705-79-0P, 11.beta.-Hydroxy-17-(difluoromethylene)-14.alpha.,15.alpha.-methyleneestra-1,3,5(10),6,8pentaen-3-yl benzoate 298705-80-3P, 14.alpha.,15.alpha.:17-Bis

## 10/748,924

methyleneestra-1,3,5(10),6,8-pentaene-3,11.alpha.-diol

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of equilenin derivs. and medicaments contg. them for hormone replacement therapy)

RN 298705-67-6 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-11,17-diol, 3',15-dihydro-3-methoxy-, diacetate, (11.alpha.,14S,15.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-68-7 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-11,17-diol, 3',15-dihydro-3methoxy-, 17-acetate, (11.alpha.,14S,15.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-69-8 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,11,17-triol, 3',15-dihydro-, (11.beta.,14S,15.beta.,17.beta.)- (9CI) (CA INDEX NAME)

RN 298705-70-1 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,11,17-triol, 3',15-dihydro-, 3-benzoate, (11.beta.,14S,15.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-71-2 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,11,17-triol, 3',15-dihydro-, 3-propanoate, (11.beta.,145,15.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-72-3 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,11,17-triol, 3',15-dihydro-, 17-decanoate, (11.beta.,145,15.beta.,17.beta.)- (9CI) (CA INDEX NAME)

RN 298705-73-4 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaen-17-one, 3',15-dihydro-3,11-dihydroxy-, (11.beta.,14S,15.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-74-5 CAPLUS

CN Cyclopropa[14,15]estra-1,3,5,7,9-pentaene-11,17-diol, 3',15-dihydro-3-methoxy-, diacetate, (11.alpha.,145,15.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-75-6 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,11,17-triol,
 3',15-dihydro-15-methyl-, (11.beta.,14S,15.beta.,17.beta.)- (9CI) (CA
 INDEX NAME)

RN 298705-76-7 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,17-diol, 11-fluoro-3',15-dihydro-, (11.beta.,14S,15.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-77-8 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaen-11-one, 3',15-dihydro-3,17-dihydroxy-, {14S,15.beta.,17.beta.} (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-78-9 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaen-11-one, 17-(acetyloxy)-3',15-dihydro-3-methoxy-, (14S,15.beta.,17.alpha.)- (9CI) (CA INDEX NAME)

RN 298705-79-0 . CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,11-diol, 17-(difluoromethylene)-3',15-dihydro-, 3-benzoate, (11.beta.,14R,15.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 298705-80-3 CAPLUS

CN Cycloprop[14,15]estra-1,3,5,7,9-pentaene-3,11-diol, 3',15-dihydro-17-methylene-, (11.alpha.,14R,15.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

## => d his

(FILE 'HOME' ENTERED AT 16:09:44 ON 10 DEC 2002)

FILE 'REGISTRY' ENTERED AT 16:09:49 ON 10 DEC 2002

L1 STRUCTURE UPLOADED

L2 6 S L1 SSS SAM

L3 STRUCTURE UPLOADED

2 S L3 SSS SAM L4

L5 16 S L3 SSS FUL

FILE 'CAPLUS' ENTERED AT 16:15:28 ON 10 DEC 2002

L6 1 S L5

FILE 'CAOLD' ENTERED AT 16:16:42 ON 10 DEC 2002

=> s 15

L7 0 L5

=> log y COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.38 149.09

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -0.62

STN INTERNATIONAL LOGOFF AT 16:16:54 ON 10 DEC 2002